

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 5.10e-01

Global applicability domain: Inside

Local applicability domain index: 5.40e-01

Confidence level: 6.85e-01

Nearest Neighbors from the Training Set

Image not found

Imazaquin

Measured: 1.86

Predicted: 5.10e-01